

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> s efaproxiral/cn

L1 1 EFAPROXIRAL/CN

=> d

THE ESTIMATED COST FOR THIS REQUEST IS 2.10 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN

RN 131179-95-8 REGISTRY

ED Entered STN: 28 Dec 1990

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)

OTHER NAMES:

CN 2-[4-[[[(3,5-Dimethylphenyl)amino]carbonyl]methyl]phenoxy]-2-methylpropionic acid

CN Efaproxiral

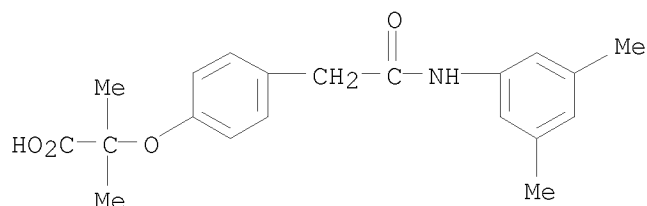
CN RSR 13

MF C20 H23 N O4

CI COM

SR CA

LC STN Files: ADISINSIGHT, ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CIN, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK*, PROMT, PROUSDDR, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

110 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

112 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

8.09

8.31

FILE 'CAPLUS' ENTERED AT 15:21:36 ON 19 MAY 2010

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 19 May 2010 VOL 152 ISS 21
 FILE LAST UPDATED: 18 May 2010 (20100518/ED)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

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        (131179-95-8 (L) PREP/RL)

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1-5 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

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10/923,271

THE ESTIMATED COST FOR THIS REQUEST IS 29.05 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1995:758997 CAPLUS
DOCUMENT NUMBER: 124:55568
ORIGINAL REFERENCE NO.: 124:10501a,10504a
TITLE: Substituted 2-methyl-2-phenoxypropionic acid
derivatives as allosteric hemoglobin modifiers to
decrease oxygen affinity in blood
INVENTOR(S): Abraham, Donald J.; Mahran, Mona; Mehanna, Ahmed;
Randad, Ramnarayan; Joshi, Gajanan S.; Panikker,
Jayashree
PATENT ASSIGNEE(S): Center for Innovative Technology, USA
SOURCE: U.S., 24 pp. Cont.-in-part of U.S. 5,290,803.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| ----- | ---- | ----- | ----- | ----- |
| US 5432191 | A | 19950711 | US 1993-101501 | 19930730 <-- |
| US 5049695 | A | 19910917 | US 1990-478848 | 19900212 <-- |
| US 5122539 | A | 19920616 | US 1991-702947 | 19910520 <-- |
| US 5382680 | A | 19950117 | US 1991-722382 | 19910626 <-- |
| US 5290803 | A | 19940301 | US 1993-6246 | 19930119 <-- |
| US 5731454 | A | 19980324 | US 1995-374206 | 19950118 <-- |
| US 5591892 | A | 19970107 | US 1995-451658 | 19950530 <-- |
| US 5648375 | A | 19970715 | US 1995-478372 | 19950607 <-- |
| US 5661182 | A | 19970826 | US 1995-478108 | 19950607 <-- |
| US 5677330 | A | 19971014 | US 1995-478371 | 19950607 <-- |
| US 5705521 | A | 19980106 | US 1995-482808 | 19950607 <-- |
| US 5927283 | A | 19990727 | US 1997-848485 | 19970508 <-- |
| US 5872282 | A | 19990216 | US 1998-41595 | 19980313 <-- |
| PRIORITY APPLN. INFO.: | | | US 1990-478848 | A2 19900212 |
| | | | US 1990-623346 | B1 19901207 |
| | | | US 1991-702947 | A2 19910520 |
| | | | US 1991-722382 | A2 19910626 |
| | | | US 1993-6246 | A2 19930119 |
| | | | US 1992-885721 | A1 19920518 |
| | | | US 1993-101501 | A2 19930730 |
| | | | US 1993-127587 | B1 19930928 |
| | | | US 1995-374206 | A3 19950118 |
| | | | US 1995-478371 | A3 19950607 |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 124:55568

AB A family of compds. R2XYZC6H4R1 where R2 is a substituted or unsubstituted aromatic compound, or a substituted or unsubstituted alkyl ring compound, or a substituted or unsubstituted phthalimide compound that incorporates X and Y where X is a carbonyl, Y is a nitrogen and R2 completes the phthalimide compound by being bonded to both X and Y, and where X, Y, and Z are CH2, NH, S, SO2, CO, O or N with the caveat that the X, Y, and Z moieties are each different from one another, and where R1 has the formula: OCR3R4CO2R5 where R1 can be connected to any position on the Ph ring, and R3 and R4

are hydrogen, halogen, Me, Et, Pr, iso-Pr, neopentyl, Bu, or substituted or unsubstituted aryl groups and these moieties may be the same or different, or alkyl moieties as part of an aliphatic ring connecting R3 and R4, and R5 is a hydrogen, halogen, C1-3 loweralkyl, or a salt cation, has been found to be useful for right-shifting Hb towards a low oxygen affinity state. The compds. are capable of acting on Hb in whole blood. In addition, the compds. can maintain the oxygen affinity in blood during storage and can restore the oxygen affinity of outdated blood. Thus, e.g., treatment of 4-HOC6H4CH2CO2H with SOCl2 and 3,5-dichloroaniline afforded the intermediate 4-HOC6H4CH2CONHC6H3Cl2-3,5; O-alkylation of the latter with acetone/CHCl3 afforded 4-(HO2CCMe2O)C6H4CH2CONHC6H3Cl2-3,5 which exhibited a P50 (mm Hg) of 87 for oxygen dissociation of normal Hb in intact human red blood cells vs. 27 for the red blood cells alone (P50 = the pressure when the scanned Hb sample is 50% saturated with oxygen).

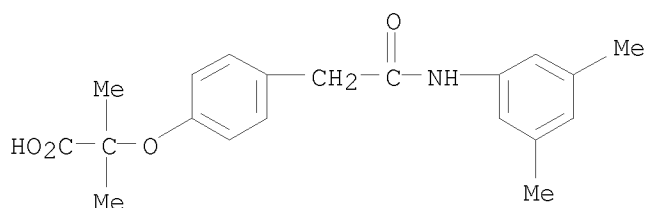
IT 131179-95-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(substituted 2-methyl-2-phenoxypropionic acid derivs. as allosteric Hb modifiers to decrease oxygen affinity in blood)

RN 131179-95-8 CAPLUS

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1993:495107 CAPLUS

DOCUMENT NUMBER: 119:95107

ORIGINAL REFERENCE NO.: 119:17137a,17140a

TITLE: Preparation of phoxymethylpropionate derivatives as allosteric hemoglobin modifiers to decrease oxygen affinity in blood

INVENTOR(S): Abraham, Donald J.; Mahran, Mona; Mehanna, Ahmed; Randad, Ramnarayan

PATENT ASSIGNEE(S): Center for Innovative Technology, USA

SOURCE: PCT Int. Appl., 67 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

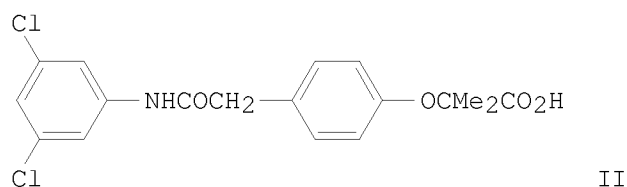
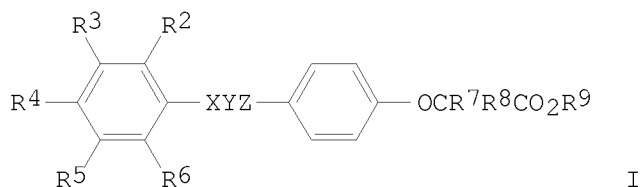
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| WO 9220335 | A1 | 19921126 | WO 1992-US4229 | 19920519 <-- |
| W: CA, JP | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE | | | | |
| US 5122539 | A | 19920616 | US 1991-702947 | 19910520 <-- |
| US 5248785 | A | 19930928 | US 1992-885721 | 19920518 <-- |
| EP 585366 | A1 | 19940309 | EP 1992-912561 | 19920519 <-- |
| EP 585366 | B1 | 20040428 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE | | | | |
| JP 07508973 | T | 19951005 | JP 1993-500270 | 19920519 <-- |
| JP 3023423 | B2 | 20000321 | | |
| CA 2109575 | C | 20000201 | CA 1992-2109575 | 19920519 <-- |
| AT 265208 | T | 20040515 | AT 1992-912561 | 19920519 <-- |
| PRIORITY APPLN. INFO.: | | | | |
| | | | US 1991-702947 | A 19910520 |
| | | | US 1992-885721 | A 19920518 |
| | | | US 1990-478848 | A2 19900212 |
| | | | WO 1992-US4229 | W 19920519 |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 119:95107

GI



AB Title compds. I (R2-R6 = H, halo, (substituted) C1-3 alkyl, C1-3 alkyl ether or ester, alkyl moieties of aromatic or aliphatic ring incorporating 2 of R2-R6 site; R7, R8 = H, Me, Et, etc.; R9 = H, halo, (substituted) C1-3 alkyl, cation salt; X, Y, Z = CH2, CO, NH, O) are prepared as allosteric Hb modifiers to decrease O affinity in blood. 4-HOC6H4CH2CO2H was refluxed with excess SOCl2, then reacted for 2 h with 3,5-Cl2C6H3NH2 to give after workup II, which showed a decrease in Hb-O affinity (i.e., increase in P50 value of 87 from control 19).

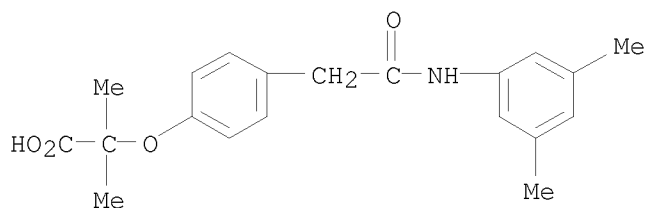
IT 131179-95-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for lowering oxygen affinity to Hb in blood)

RN 131179-95-8 CAPLUS

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-

methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1993:45721 CAPLUS

DOCUMENT NUMBER: 118:45721

ORIGINAL REFERENCE NO.: 118:8119a,8122a

TITLE: Allosteric hemoglobin modifiers useful for decreasing
oxygen affinity and preserving oxygen carrying
capability of stored blood

INVENTOR(S): Abraham, Donald J.; Mahran, Mona; Mehanna, Ahmed;
Randad, Ramnarayan

PATENT ASSIGNEE(S): Center for Innovative Technology, USA

SOURCE: U.S., 20 pp. Cont.-in-part of U.S. 5,049,695.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| US 5122539 | A | 19920616 | US 1991-702947 | 19910520 <-- |
| US 5049695 | A | 19910917 | US 1990-478848 | 19900212 <-- |
| CA 2051693 | A1 | 19910813 | CA 1991-2051693 | 19910206 <-- |
| CA 2051693 | C | 20050607 | | |
| US 5248785 | A | 19930928 | US 1992-885721 | 19920518 <-- |
| WO 9220335 | A1 | 19921126 | WO 1992-US4229 | 19920519 <-- |
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| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE | | | | |
| EP 585366 | A1 | 19940309 | EP 1992-912561 | 19920519 <-- |
| EP 585366 | B1 | 20040428 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE | | | | |
| JP 07508973 | T | 19951005 | JP 1993-500270 | 19920519 <-- |
| JP 3023423 | B2 | 20000321 | | |
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| EP 1236711 | A2 | 20020904 | EP 2002-12781 | 19920519 <-- |
| EP 1236711 | A3 | 20020918 | | |
| EP 1236711 | B1 | 20040303 | | |
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| AT 265208 | T | 20040515 | AT 1992-912561 | 19920519 <-- |

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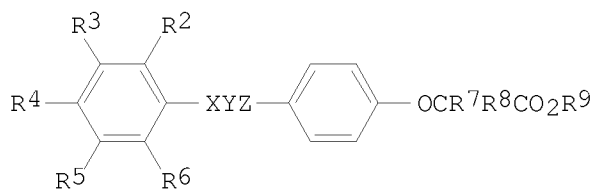
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| EP 1468680 | A2 | 20041020 | EP 2004-9908 | 19920519 | <-- |
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| ES 2220857 | T3 | 20041216 | ES 2002-12781 | 19920519 | <-- |
| ES 2223042 | T3 | 20050216 | ES 1992-912561 | 19920519 | |
| US 5250701 | A | 19931005 | US 1993-6378 | 19930119 | <-- |
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| US 5661182 | A | 19970826 | US 1995-478108 | 19950607 | <-- |
| US 5677330 | A | 19971014 | US 1995-478371 | 19950607 | <-- |
| US 5705521 | A | 19980106 | US 1995-482808 | 19950607 | <-- |
| US 5927283 | A | 19990727 | US 1997-848485 | 19970508 | <-- |

PRIORITY APPLN. INFO.:

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| US 1991-702947 | A2 | 19910520 |
| US 1991-722382 | A2 | 19910626 |
| US 1992-885721 | A | 19920518 |
| EP 1992-912561 | A3 | 19920519 |
| WO 1992-US4229 | W | 19920519 |
| US 1993-6246 | A2 | 19930119 |
| US 1993-101501 | A2 | 19930730 |
| US 1993-127587 | B1 | 19930928 |
| US 1995-374206 | A3 | 19950118 |
| US 1995-478371 | A3 | 19950607 |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 118:45721
GI



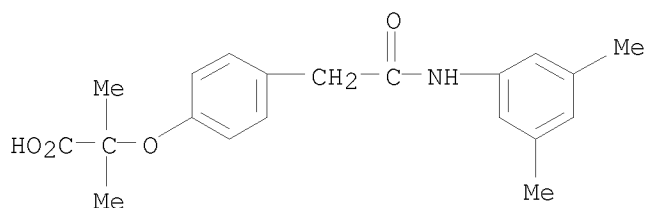
I

AB I (X,Y,Z = CH₂, NH or O and R²-R⁶ = e.g., H, halo, substituted or unsubstituted C1-3 allyl, R⁷, R⁸ = H, Me or Et, R⁹ = H, alkyl, or metal salt) are prepared and have the ability to maintain oxygen affinity in blood during storage and can restore the O affinity of outdated blood.
p-Acetaminophenol was treated with acetone and CHCl₃ in NaOH solution and the acetaminophenoxymethylpropionic acid obtained after acidification was hydrolyzed and later acylated with an acid chloride such as phenylacetyl chloride. The compds. showed O carrying properties of stored blood.

IT 131179-95-8P
RL: PREP (Preparation)
(preparation of, as allosteric Hb modifier for decreasing oxygen affinity

10/923,271

and preserving oxygen carrying properties)
RN 131179-95-8 CAPLUS
CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)



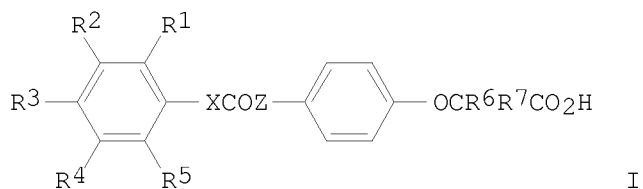
OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS
RECORD (40 CITINGS)
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1991:655817 CAPLUS
DOCUMENT NUMBER: 115:255817
ORIGINAL REFERENCE NO.: 115:43485a, 43488a
TITLE: Preparation of allosteric hemoglobin modifiers
INVENTOR(S): Abraham, Donald J.; Mehanna, Ahmed; Randad,
Ramnarayan; Mahran, Mona
PATENT ASSIGNEE(S): Center for Innovative Technology, USA
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| ----- | ---- | ----- | ----- | ----- |
| WO 9112235 | A1 | 19910822 | WO 1991-US833 | 19910206 <-- |
| W: CA, JP | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE | | | | |
| US 5049695 | A | 19910917 | US 1990-478848 | 19900212 <-- |
| CA 2051693 | A1 | 19910813 | CA 1991-2051693 | 19910206 <-- |
| CA 2051693 | C | 20050607 | | |
| EP 471811 | A1 | 19920226 | EP 1991-904612 | 19910206 <-- |
| EP 471811 | B1 | 19951227 | | |
| R: DE, FR, GB, IT | | | | |
| JP 04506812 | T | 19921126 | JP 1991-504932 | 19910206 <-- |
| JP 3023422 | B2 | 20000321 | | |

PRIORITY APPLN. INFO.: US 1990-478848 A 19900212
WO 1991-US833 W 19910206

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 115:255817; MARPAT 115:255817
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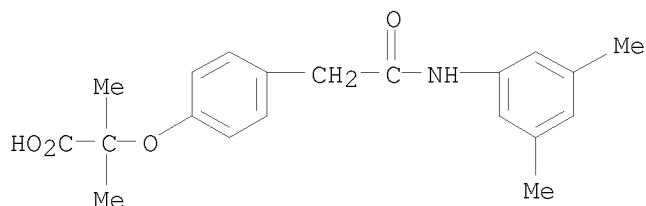


AB Title modifiers I [R1 - R5 = H, halo, (substituted) C1-3 alkyl; R6, R7 = H, Me; X, Z = CH2, NH, O, with the proviso that when X is CH2, Z is NH, when X is NH, Z is either CH2 or O, and when X is O, Z is NH] are prepared NaOH was added to p-(AcNH)C6H4OH in acetone, followed by addition of CHCl3, to give after acidification with HCl the appropriate (acetaminophenoxy)methylpropionic acid, which was treated with KOH to give 4-(H2N)C6H4OCMe2CO2H, which was dissolved with stirring in aqueous NaOH, and to this solution was added PhCH2COCl to give I (R1-R5 = H, R6 = R7 = Me, X = CH2, Z = NH) (II). The biol. activities of II and addnl. I are given.

IT 131179-95-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as allosteric Hb modifier)

RN 131179-95-8 CAPLUS

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1991:81170 CAPLUS

DOCUMENT NUMBER: 114:81170

ORIGINAL REFERENCE NO.: 114:13837a,13840a

TITLE: Allosteric modifiers of hemoglobin. 1. Design, synthesis, testing, and structure-allosteric activity relationship of novel hemoglobin oxygen affinity decreasing agents

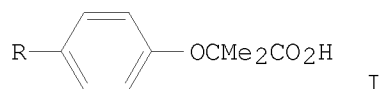
AUTHOR(S): Randad, Ramnarayan S.; Mahran, Mona A.; Mehanna, Ahmed S.; Abraham, Donald J.

CORPORATE SOURCE: Dep. Med. Chem., Virginia Common. Univ., Richmond, VA, 23298-0581, USA

SOURCE: Journal of Medicinal Chemistry (1991), 34(2), 752-7
CODEN: JMCMAR; ISSN: 0022-2623

10/923,271

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:81170
GI

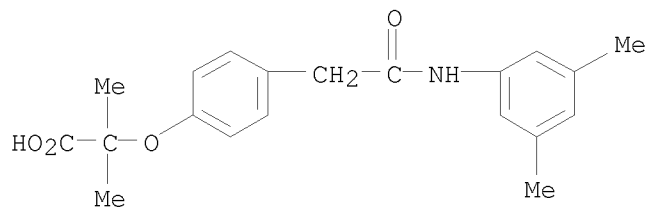


AB Three isomeric series of 2-aryloxy-2-methylpropionic acids I (R = R1CH2CONH, R1CONHCH2, R1NHCOCH2; R1 = Ph, substituted phenyl) were prepared and studied for their ability to decrease the oxygen affinity of human Hb A. Structure-activity relationships are presented. Several of the new compds. were strong allosteric effectors of Hb. The two most active compds. are I (R = 3,5-R22C6H3NHCCH2; R2 = Cl, Me) (II). Compared to other known potent allosteric effectors, II show greater activity. II also exhibit a right shift in the oxygen equilibrium curve when incubated with whole blood.

IT 131179-95-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as allosteric effector of Hb)

RN 131179-95-8 CAPLUS

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 44 THERE ARE 44 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)

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